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BOOK OF ABSTRACTS

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Interaction and dynamic between rare gases and 2d layered materials

J. Campos-Martínez, M. I. Hernández, M. Bartolomei

Instituto de Física Fundamenal (IFF-CSIC)

Serrano 123, E-28006 Madrid, SPAIN

The interaction of atoms and molecules with carbonaceous layered materials is a topic of interest both from a fundamental and a more applied points of view.

We have been recently working on the construction of reliable global potential energy surfaces for these systems and their application in different dynamical processes. There is an ample literature in which these processes are studied by Molecular Dynamics (MD) simulations and/or approximate quantum models. In this contribution we report three-dimensional wave packet calculations to study the interaction potential between graphene and graphite with rare gas atoms as well as the transport of {4,3}^He atoms through a periodic rigid mebrane of graphdiyne -a novel material composed of nanopores at regular distances- and also through a holey graphene model (with a force-field based on simple Lennard- Jones interactions). A good agreement is found between approximate quantum models and present calculation for the case of graphdiyne, with a much more pronounced differences for the transmission through nanoporous graphene.

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